Drug Metabolism and Disposition

A PREDICTIVE LIGAND-BASED BAYESIAN MODEL FOR HUMAN DRUG INDUCED LIVER INJURY

Sean Ekins, Antony J. Williams and Jinghai J. Xu

Collaborations in Chemistry, 601 Runnymede Avenue, Jenkintown, PA 19046, U.S.A. (SE)

Department of Pharmaceutical Sciences, University of Maryland, MD 21201, U.S.A. (SE)

Department of Pharmacology, University of Medicine & Dentistry of New Jersey (UMDNJ)-Robert Wood Johnson Medical School, 675 Hoes Lane, Piscataway, NJ 08854. (SE)

Royal Society of Chemistry, 904 Tamaras Circle, Wake Forest, NC-27587. (AJW)

Merck & Co., Inc., 126 E. Lincoln Ave, Rahway, NJ 07065. (JJX)

Supplemental Figure 1.

PCA analysis for DILI combined training and test set compared with a set of 77 recently approved drugs.

532 compounds in the DILI training and test set (N= 532, blue) were compared with 77 recently approved drugs obtained from the Prous database. The following descriptors were used with Discovery Studio 2.5.5: ALogP, molecular weight, number of hydrogen bond donors, number of hydrogen bond acceptors, number of rotatable bonds, number of rings, number of aromatic rings, and molecular fractional polar surface area. 0.83 % of the variance was explained with the first three principal components. One outlier approved drug molecule is Sugammadex (bottom, yellow).